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STRUCTURE FILE UPDATES: 6 NOV 2007 HIGHEST RN 952567-23-6

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STRUCTURE FILE UPDATES: 6 NOV 2007 HIGHEST RN 952567-23-6 DICTIONARY FILE UPDATES: 6 NOV 2007 HIGHEST RN 952567-23-6

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

```
http://www.cas.org/support/stngen/stndoc/properties.html
=> s 105816-04-4/rn
             1 105816-04-4/RN
L1
=> d
     ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
L1
     105816-04-4 REGISTRY
RN
ED
     Entered STN: 21 Dec 1986
     D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]- (CA
     INDEX NAME)
OTHER CA INDEX NAMES:
     D-Phenylalanine, N-[[4-(1-methylethyl)cyclohexyl]carbonyl]-, trans-
CN
     (-)-N-[(trans-4-Isopropylcyclohexyl)carbonyl]-D-phenylalanine
CN
     A 4166
CN
     AY 4166
CN
     D-Nateglinide
CN
     DJN 608
CN
     Fastic
CN
     Glinate
     Nateglinide
CN
CN
     Natelide
CN
    SDZ-DJN 608
     Senaglinide
CN
     Starlix
CN
     Starlix DS
CN
CN
     Starsis
     STEREOSEARCH
FS
DR
     418766-62-8
MF
     C19 H27 N O3
CI
     COM
SR
     CA
LC.
     STN Files:
                  ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BIOSIS, BIOTECHNO,
       CA, CABA, CAPLUS, CASREACT, CBNB, CHEMCATS, CIN, CSCHEM, DDFU, DRUGU,
       EMBASE, IMSCOSEARCH, IMSDRUGNEWS, IMSPATENTS, IMSRESEARCH, IPA, MEDLINE,
       MRCK*, PATDPASPC, PHAR, PIRA, PROMT, PROUSDDR, PS, RTECS*, SCISEARCH,
       SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL
```

(*File contains numerically searchable property data)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ & & & \\ Ph & & & \\ \hline & & & \\ CO_2H & O & \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

596 REFERENCES IN FILE CA (1907 TO DATE)

11 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

598 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> str 105816-04-4

:

:

:end

L2 STRUCTURE CREATED

=> s 12 fam full

L3 895860 12

=> s 12 fam full

FULL SEARCH INITIATED 16:31:21 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 441 TO ITERATE

100.0% PROCESSED 441 ITERATIONS

36 ANSWERS

SEARCH TIME: 00.00.01

L4 36 SEA FAM FUL L2

=> d scan

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[4-(1-methylethyl)cyclohexyl]carbonyl]- (9CI)

MF C19 H27 N O3

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ & & & \\ Ph & & & \\ \hline & & & \\ CO_2H & O \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):36

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

MF C19 H27 N O3 . H2 O

Absolute stereochemistry.

H20

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IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-,
hydrochloride (2:1), hydrate (2:1) (9CI)

MF C19 H27 N O3 . 1/2 C1 H . 1/2 H2 O

Absolute stereochemistry.

●1/2 HCl

●1/2 H₂O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd. with 2A,2B,2C,2D,2E,2F,2G,3A,3B,3C,3D,3E,3F,3G,6A,6B,6C,6D,6E,6F,6G-heneicosa-O-ethyl- β -cyclodextrin (1:1) (9CI)

MF C84 H154 O35 . C19 H27 N O3

CM 1

PAGE 2-A

CM 2

Absolute stereochemistry.

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd. with β -cyclodextrin (1:1) (9CI)

MF C42 H70 O35 . C19 H27 N O3

CM 1

Absolute stereochemistry.

PAGE 1-A

Н

PAGE 2-A

- L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
- IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd. with 2A,2B,2C,2D,2E,2F,2G,6A,6B,6C,6D,6E,6F,6G-tetradeca-O-ethyl- β -cyclodextrin (1:1) (9CI)
- MF C70 H126 O35 . C19 H27 N O3

CM 1

PAGE 2-A

CM 2

Absolute stereochemistry.

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd. with 2A,2B,2C,2D,2E,2F,2G,3A,3B,3C,3D,3E,3F,3G,6A,6B,6C,6D,6E,6F,6G-heneicosa-O-methyl- β -cyclodextrin (1:1) (9CI)

MF C63 H112 O35 . C19 H27 N O3

CM 1

Absolute stereochemistry.

PAGE 1-A

H OMe

PAGE 2-A

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IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd. with 2A,2B,2C,2D,2E,2F,2G,6A,6B,6C,6D,6E,6F,6G-tetradeca-O-methyl- β -cyclodextrin (1:1) (9CI)

MF C56 H98 O35 . C19 H27 N O3

CM 1

Absolute stereochemistry.

PAGE 1-A

OMe

PAGE 2-A

36 ANSWERS L4REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd. with β -cyclodextrin (2:1) (9CI) C42 H70 O35 . 2 C19 H27 N O3

MF

CM 1

Absolute stereochemistry.

PAGE 1-A

Н

PAGE 2-A

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd. with $\beta\text{-cyclodextrin}$ (3:1) (9CI)

MF C42 H70 O35 . 3 C19 H27 N O3

CM 1

Absolute stereochemistry.

PAGE 1-A

Н

PAGE 2-A

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IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd. with heptane (9CI)

MF C19 H27 N O3 . x C7 H16

CM 1

 $Me^-(CH_2)_5-Me$

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IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd.
with trichloromethane (9CI)

MF C19 H27 N O3 . x C H C13

CM 1

Absolute stereochemistry.

CM 2

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd.
with 1,2-dichloroethane (9CI)

MF C19 H27 N O3 . x C2 H4 C12

CM 1

 $Cl - CH_2 - CH_2 - Cl$

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd. with tetrachloromethane (9CI)

MF C19 H27 N O3 . x C C14

CM 1

Absolute stereochemistry.

CM 2

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd.
with dimethylbenzene (9CI)

MF C19 H27 N O3 . x C8 H10

CM 1

Absolute stereochemistry.

CM 2

2 (D1-Me)

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd. with 1,2-dimethoxyethane (9CI)

MF C19 H27 N O3 . x C4 H10 O2

CM 1

Absolute stereochemistry.

CM 2

 ${\tt MeO-CH_2-CH_2-OMe}$

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd. with N,N-dimethylformamide (9CI)

MF C19 H27 N O3 . x C3 H7 N O

CM 1

Absolute stereochemistry.

CM 2

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd. with 1-methyl-2-pyrrolidinone (9CI)

MF C19 H27 N O3 . x C5 H9 N O

CM 1

Absolute stereochemistry.

CM 2

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd. with N,N-dimethylacetamide (9CI)

MF C19 H27 N O3 . x C4 H9 N O

CM 1

Absolute stereochemistry.

CM 2

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd.
with 1-propanol (9CI)

MF C19 H27 N O3 . x C3 H8 O

CM 1

Absolute stereochemistry.

CM 2

 $_{\rm H3C-CH2-CH2-OH}$

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd.
with 1-butanol (9CI)

MF C19 H27 N O3 . \times C4 H10 O

CM 1

Absolute stereochemistry.

CM 2

 $_{\rm H3C-CH_2-CH_2-CH_2-OH}$

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd.
with ethanol (9CI)

MF C19 H27 N O3 . x C2 H6 O

CM 1

 $_{\rm H3C-CH2-OH}$

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd.
with methanol (9CI)

MF C19 H27 N O3 . x C H4 O

CM 1

Absolute stereochemistry.

CM 2

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L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-,
 ammonium salt (9CI)

MF C19 H27 N O3 . x H3 N

Absolute stereochemistry.

●x NH3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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MF C19 H27 N O3 . 1/2 Ca

Absolute stereochemistry.

●1/2 Ca

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-,
monopotassium salt (9CI)

MF C19 H27 N O3 . K

Absolute stereochemistry.

K

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

MF C19 H27 N O3 . Na

Na

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd.
with L-lysine (1:1) (9CI)

MF C19 H27 N O3 . C6 H14 N2 O2

CM 1

Absolute stereochemistry.

CM 2

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI)

MF C19 H27 N O3 . C4 H11 N O3

CM 1

$$\begin{array}{c} {\rm NH_2} \\ | \\ {\rm HO-CH_2-C-CH_2-OH} \\ | \\ {\rm CH_2-OH} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-, compd. with 1-deoxy-1-(methylamino)-D-glucitol (1:1) (9CI)

MF C19 H27 N O3 . C7 H17 N O5

CM 1

Absolute stereochemistry.

CM 2

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-

MF C19 H27 N O3

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl-14C]-(9CI)

MF C19 H27 N O3

Absolute stereochemistry.

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MF C19 H27 N O3 . x H2 O

Absolute stereochemistry.

●x H2O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN D-Phenylalanine, N-[[cis-4-(1-methylethyl)cyclohexyl]carbonyl]- (9CI)

MF C19 H27 N O3

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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IN L-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]- (9CI)

MF C19 H27 N O3

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L4 36 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN D-Phenylalanine, N-[[trans-4-(1-methylethyl)cyclohexyl]carbonyl]-

MF C19 H27 N O3

CI COM

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED